

Bruker / MIT Symposium 2024

JUDGING DATA QUALITY IN RECIPROCAL SPACE

Ashley Weiland, Bruker AXS LLC ashley.weiland@bruker.com

Is this crystal worth collecting on? Is my unit cell correct? Is there twinning lurking in my data? These single crystal X-ray diffraction questions can be addressed with the help of a reciprocal lattice viewer. A feature within APEX5, View Reciprocal Lattice aids in determining key crystallographic parameters such as unit cell dimensions, symmetry operations, and potential twinning or modulation effects. This talk will focus on navigating the View Reciprocal Lattice plug-in in APEX5 and will highlight strategies to address complex crystallographic challenges including twinning and modulation.